SN S-96,583
Docket No 10/017,643
In Response to Office Action dated September 24, 2003

AMENDMENTS TO THE CLAIMS:

This listing of claims will replace all prior versions, and listings, of claims in the application:

LISTING OF CLAIMS:

1. (Currently Amended)   A method for improving an electron density map representing a crystal structure comprising:

(a)   obtaining by x-ray diffraction observed structure factor amplitudes for a plurality of reflections from the crystal structure;

(b)   selecting a starting set of crystallographic phases to combine with the observed structure factor amplitudes to form a first set of structure factors;

(c)   deriving a first electron density map from the first set of structure factors;

(d)   identifying features of the first electron density map to obtain expected distributions of electron density;

(e)   making a comparison between the first electron density map and the expected distribution of electron density;

(f)   estimating how changes in the crystallographic phase of a reflection k affect the comparison;

(g)   establishing crystallographic phase probability distributions from the comparisons for the possible crystallographic phases of reflection k;

(h)   repeating steps (c) through (g) as k is indexed through all of the plurality of reflections;

(i)   deriving an updated electron density map using crystallographic phases determined to be most probable from the crystallographic phase probability distributions for each one of the reflections; and

(j)   repeating steps (d) through (i) to obtain a final set of crystallographic phases with minimum bias from known electron density maps; and

(k)   forming a final electron density map using the final set of crystallographic phases.

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2. (Original)   The method of Claim 1, wherein identifying features of the electron density map includes making probability estimates of whether each point in the map is located in a solvent region or a crystal structure region.

3. (Original)   The method of Claim 1, wherein identifying features of the election density map includes estimates of whether the electron density at each point in the map is related by non-crystallographic symmetry to electron density at another point in the map.

4. (Original)   The method of Claim 1, includes estimates of whether a structural motif is located at each point in the map.

5. (Original)   The method of Claim 4, wherein the structural motif is a helix.

6. (Original)   The method of any one of Claims 1, 2, 3, or 4, wherein the crystallographic phase probability distributions are log-likelihood functions.

7. (Original)   The method of Claim 1, further including the steps of calculating first and second derivatives for the crystallographic phase probability distributions with respect to the structure factors; and

applying an FFT-based algorithm to determine the most probable crystallographic phase probability distributions.

8. (Original)   The method of Claim 1, wherein the step of selecting a starting set of crystallographic phases includes:

selecting a model crystal structure having similarities to the crystal structure being examined;

assigning a low weighting factor to structure factors of the model crystal structure; and

combining the weighted structure factors with the observed structure factors for deriving the first electron density map.

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